**Integrated Programme for Better Air Quality (IBAQ Programme)**

# CITY SOLUTIONS TOOLKIT:

# AIR QUALITY MODELING CONCEPTS AND PROCESS

## BACKGROUND

Air quality management is not limited to collecting air quality monitoring data and other information through emission inventories (EIs). One of the common and main challenges in cities is that there is not enough resources and available data to 'tell the full story' or give the complete picture on where air pollutants come from or where they can go, as well as what would be their possible impacts. Studies on the environment are generally complex, and much more so for atmospheric or air pollution studies in a given location with unique population and geographical characteristics.

Air quality managers can turn to air quality modeling to arrive at rational decision making, to augment data that cannot be currently or immediately obtained, or to complement data that has already been collected. In this module, the basic principles and considerations in performing an air quality modeling is discussed, to guide the reader in understanding its advantages in air quality management. Further, it can help in making the necessary preparations for running an air quality model.

Modeling is a method to give a representation of reality that is often difficult to understand. Models help in simplifying situations by integrating actual data with assumptions that best fit the context of the area under study. In the same way a picture is a representation of the subject, air quality modeling is a representation of what is happening to the air quality of an area. This document introduces modeling concepts and stages of performing this technique, to familiarize the reader on the advantages of this component of air quality management.

## INTRODUCTION

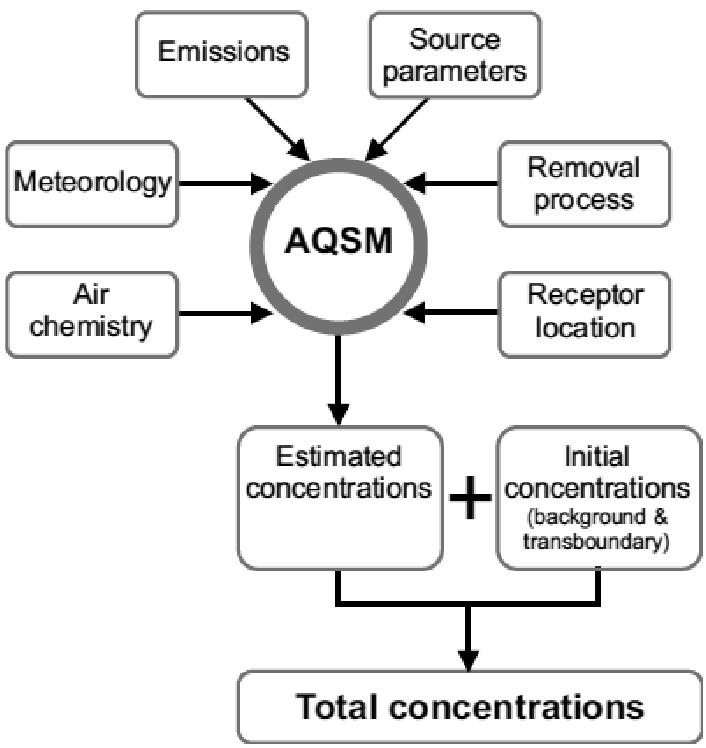
Just like any tool, models make it easier to apply effective management of air quality. This is done through complex calculations with the use of assumptions to give an estimate and prediction of what the situation will be. An air quality simulation model (AQSM) is a numerical technique or methodology for estimating air pollutant concentrations in space and time. It is a function of the spatial distribution of sources and the existing meteorological and topographical conditions.

If the output of the model is validated, then key decisions can be made (refer to module on Application of Air Quality Modeling in Policy Development). Time, effort, and cost can go down if proper models are used and implemented by experts in the field. The outcomes can be used to further determine how a certain action, project, measure, or policy can impact the quality of air, through calculations made considering various scenarios.

Air quality modeling can yield air pollutant concentrations per grid, which can be as small as a 200 meter-size area or less. This means having air pollutant values every 200 meters, which, if obtained by a very dense monitoring network can be very expensive. Assuming that infrastructure and technical capacity (refer to module on Air Quality Modeling Tools for more details) are already in place, modeling can be less costly compared to extensive ground-based air pollutant monitoring. It can also be a proactive way of preventing negative implications of emission sources to air quality since projections can be made which consider ongoing or future activities and actions.

## AIR QUALITY MODELING CONCEPTS

The basic components of an AQSM is described in the diagram below. This can give a snapshot of what input data may be needed (refer to module on Air Quality Modeling: Data Needs and Operational Guidelines for complete discussion of data input needs).




Source: Adapted from Clean Air Asia, 2019

The major categories of air quality models are summarized below (Clean Air Asia and UN Environment, 2019; US EPA, 2017):

**Source-based/Dispersion Models** - Estimates the concentration of pollutants at specified ground-level monitoring sites surrounding a source. This provides an idea of how much pollution is received in relation to the source. Through mathematical calculations, the model characterizes the atmospheric conditions that disperse or 'spread' pollutants from a single or several emission sources.

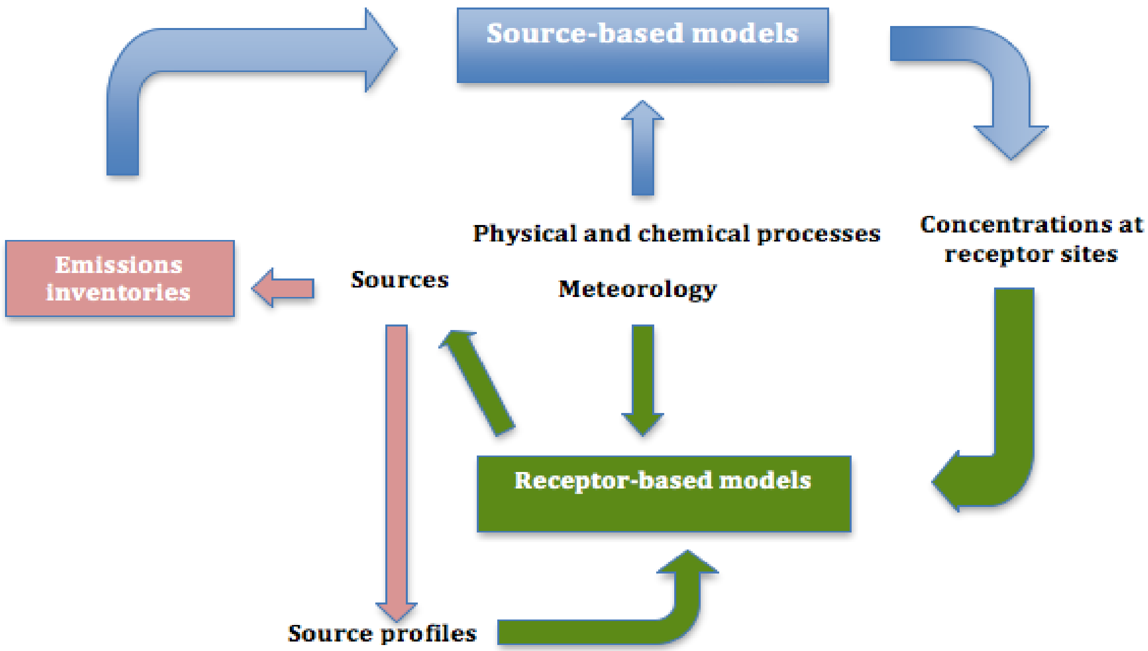
Requirements: Meteorological data, geophysical data, software/equations, emissions data
General use: For permitting, to determine the extent of dispersion of emissions, and for checking compliance to air quality standards

**Receptor Models/Source Apportionment (SA) Models** – Determines the contribution (fraction, percentage or portion) of specific sources on the quality of air measured at specific sites, location/s of interest or 'receptors'. The air quality at a particular location and time is possibly composed of several air pollutants, due to many sources. Through the model, estimations are done to identify which sources have more contributions to the mix of pollutants measured. At the receptor site, the chemical and physical characteristics of gases and particles measured are analyzed together with samples collected in the site nearest to the source.

Requirements: Laboratory analysis of chemical compositions (usually done through chemical analysis of filters), source information (technology and pollutants emitted)
General use: To determine sources to be prioritized in an area; to develop and inform control strategies and other measures to address source.

In dispersion modeling, the questions of "what happens to the emissions, where does it go?" are answered. For receptor modeling, the questions answered are "where did this come from, how much of the pollutants here come from this (particular) source?"

Both models use knowledge of emission sources that contribute to pollutant concentrations in a specific location. The source-oriented approach starts from an EI and uses source-oriented models (dispersion models) in the form of chemical transport models to estimate the contribution of each source at a receptor location. Source profiles and EIs (refer to module on Development of source and emissions database for more details) thus play a key role in air quality dispersion modeling, as well as meteorological data, and processes (physical, chemical) that affect air pollutants. The following figure shows the flow of information on dispersion (source-based) and receptor-based modeling.




Source: Clean Air Asia, 2019

**Photochemical Models** – Another type of air quality modeling which estimates and simulates how pollutant concentrations change in the atmosphere. The model is capable of taking into account the chemical reactions that take place as pollutants get dispersed in the air, with specific influence of sunlight-induced reactions, and other physical and chemical processes. These can be applied at varying scales, from local, to regional, national, and global. Compared to dispersion and receptor modeling, photochemical models have better ability to fully characterize physical conditions in the atmosphere, provide more complex simulations, and thus predict species concentrations. The data requirements and general use are similar to both dispersion and receptor modeling, but more complex.

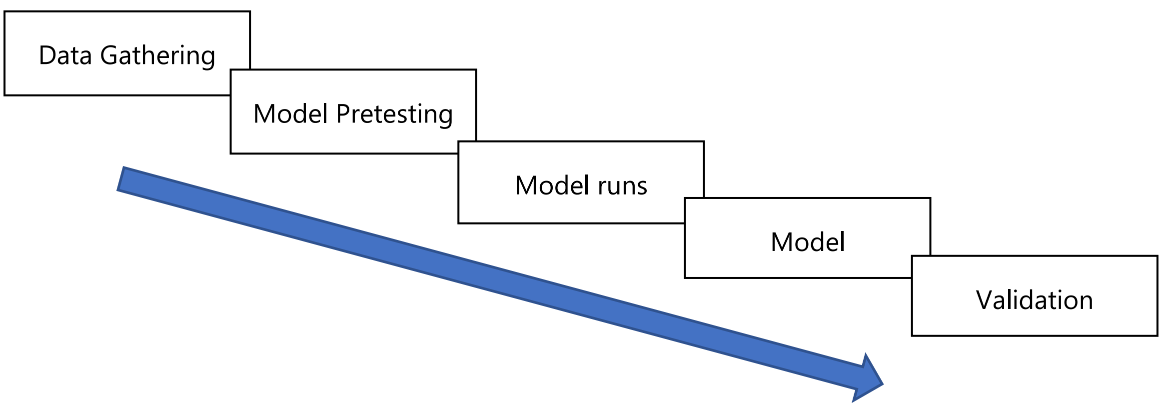
To highlight what can be achieved through air quality modeling in comparison with air quality monitoring, a table summary is presented below (Clean Air Asia and UN Environment, 2019):

| **Task** | **Monitoring capability** | **Modeling capability** |
|---|---|---|
| *to be undertaken* | *for undertaking the task* | |
| Spatial distributions | Yes, but only cost-effective if passive or low-cost monitors are used | Yes |
| Temporal distributions | Yes, if automatic continuous monitors are employed or time resolution is sufficient | Yes, if continuous emission date and meteorological field data are available |
| Source apportionment, source-oriented | No | Yes |

| | | |
|---|---|---|
| Source apportionment, receptor-oriented | Yes, if receptor monitoring and modeling are applied simultaneously | |
| "Exotic" compounds (e.g. gaseous mercury) | No if monitoring methodology does not exist or is too expensive | Yes |
| Hotspot determination | Yes, with sufficient a-priori knowledge | Yes |
| Forecasting air quality | No | Yes |
| Estimating outdoor exposures | Yes, if personal monitors are applied | Yes, if time pattern of human activities is available |
| Estimating indoor exposures | Yes, if personal monitors are applied | No |

## AIR QUALITY MODELING PROCESS

The process of air pollution modeling in general contains five stages described below. Familiarity with the process can help in preparing the necessary data for each step.




1. **Data gathering for input**
   The data input for air quality modeling refers to all important information that must be collected, compiled and fed to the model (please refer to module on Air Quality Modeling: Data Needs and Operational Guidelines for more details).

2. **Model Pretesting**
   In case the specific model (tool) has not been used yet by any of the modelers or members of the working group, trial runs in the model can be done using established data from previous studies. This is to check for possible challenges in using the tool.

3. **Model Runs**
   a. Dispersion calculations

   In this stage, estimations are done on how pollutants are dispersed, transported, or 'moving' from the emission source/s.

   b. Deriving concentrations

Given the dispersion of the pollutants in the study area with respect to meteorological and geographical conditions, the model calculates for the ambient air quality or the concentration of pollutants in specified locations or spatial grids.

4. **Model Output/Processing or Analysis of results**

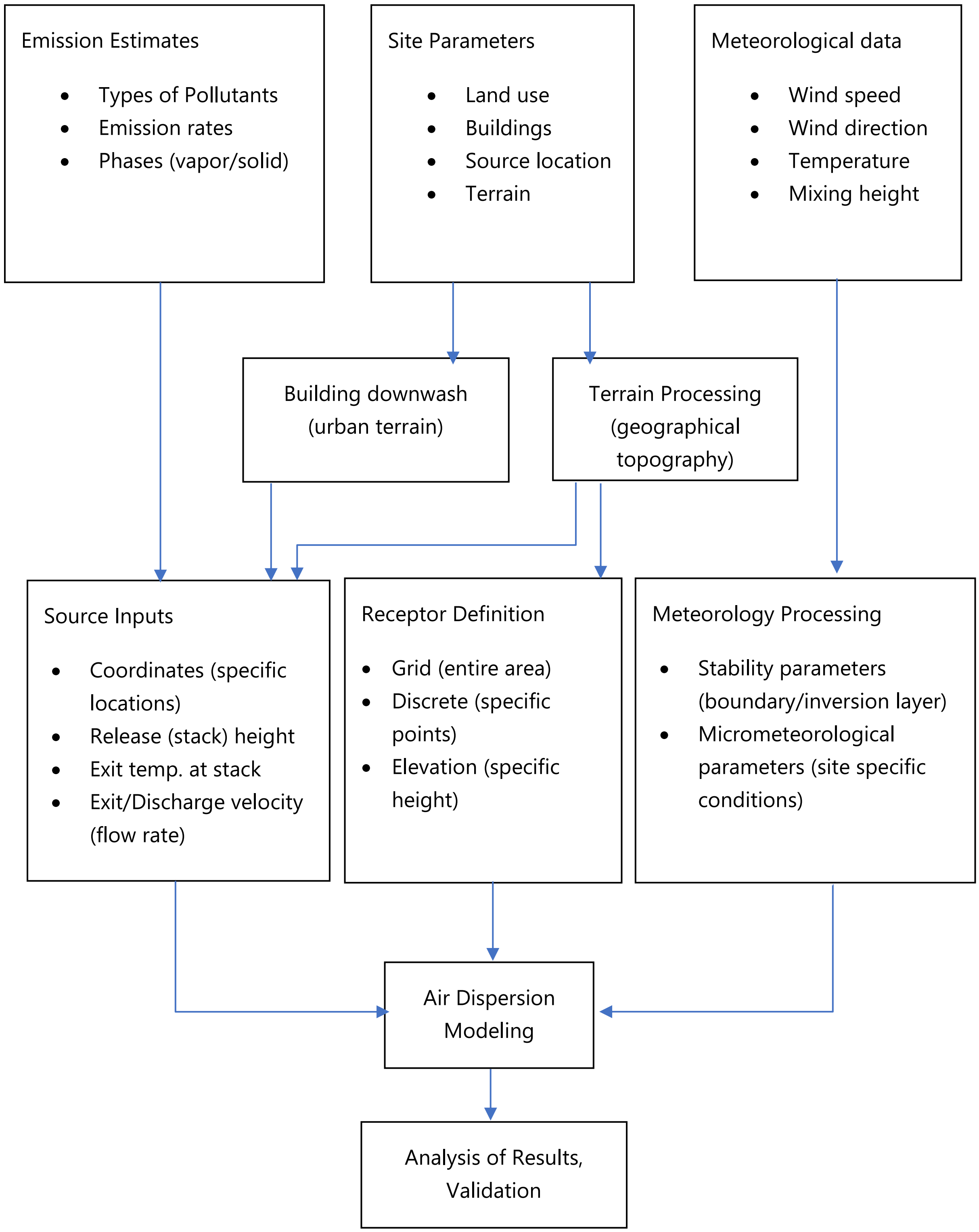
   The resulting data on emissions or/and ambient air quality is compared versus national or local standards and air quality guideline values for compliance checking.

5. **Validation or 'Ground truthing'**

   Checking with experts or confirmation of concentration output with actual air quality monitoring instruments or filter samples.

Some of the stages may take time to accomplish. But generally, this kind of work requires three months to a year. Most of the time will be spent on data gathering and data validation. Model pretesting is a step to ensure that the appropriate resources have been considered so that the model and subsequent analysis can be accomplished. Multiple runs of the model are suggested as well as critical work on refining the output of the model during the processing stage. Before the output of the model can be considered as reliable, validation must be done.

For dispersion modeling, the figure below presents the process, with suggested general data considerations for input (modified from Clarke, 2006). As discussed, there should be adequate information from the sources of emissions, meteorological data and the actual study site.


Emission Estimates
Types of Pollutants
Emission rates
Phases (vapor/solid)
Site Parameters
Land use
Buildings
Source location
Terrain
Meteorological data
Wind speed
Wind direction
Temperature
Mixing height
Building downwash (urban terrain)
Terrain Processing (geographical topography)
Source Inputs
Coordinates (specific locations)
Release (stack) height
Exit temp. at stack
Exit/Discharge velocity (flow rate)
Receptor Definition
Grid (entire area)
Discrete (specific points)
Elevation (specific height)
Meteorology Processing
Stability parameters (boundary/inversion layer)
Micrometeorological parameters (site specific conditions)
Air Dispersion Modeling
Analysis of Results, Validation

Another important note before performing the air quality modeling is to check if there are existing policies or air quality guidelines implemented by the government or the Ministry of Environment. In some cases, only specific models are recognized or recommended for use, for uniformity and coherence with pre-existing modeling efforts. This is important because it will inform the entire process on what model to use, what data to input, and what objectives to meet for air quality management.

The typical modeling process would require a few months to complete if data access is not an issue. In some cases, data and result validation takes time, as well as the discussion and the use of the results. It is suggested that other resources such as the Air Quality Modeling Tools for Cities should also be studied to understand most of the processes and details of this document, while the module on Air Quality Modeling: Data Needs and Operational Guidelines should be referred to for the final consideration in efficiently preparing for and performing this AQM component. The module on Application of Air Quality Modeling Results in Policy Development, on the other hand, can be referred to for guidance on how to use air quality modeling outcomes for policy formulation.

## REFERENCES:

Clarke, Bruce. 2009. Training on Air Quality Modeling. Sinclair Knight Merz, Manila, Philippines. Sponsored by the Philippine government Department of Environment and Natural Resources – Environmental Management Bureau.

Clean Air Asia and UN Environment. 2019. Guidance Framework for Better Air Quality in Asian Cities: Guidance Area 2: Emissions Inventory and Modeling.

SEI, 2008. Foundation Course on Air Quality Management in Asia: Modeling. Edited by: Gary Haq and Dieter Schwela. Stockholm Environment Institute.

US EPA. 2017. Air Quality Models. Accessed from https://www.epa.gov/scram/air-quality-models